1 The one-dimensional case

The Laplace approximation is a versatile tool that can be used to approximate integrals of the form

$$\int_a^b \exp[-Mf(x)]dx \tag{1}$$

The basic assumption is that the largest contribution value to the integral is in an interval around the critical points of $f(x)$. Under the laplace approximation, it is a ssumed that the value of f(x) 'far away' from the critical point is so low, that it effectively does not contribute to the total integral. The integration limits will thus be replaced as shown below.

Approximate $f(x)$ by the Taylor series

$$f(x) \approx f(x_0) + (x - x_0)f'(x_0) + \frac{1}{2}(x - x_0)^2 f''(x_0) + O \tag{2}$$

The Tailor series for $f(x)$ around the critical point, is then

$$f(x) \approx f(x_0) + \frac{1}{2}(x - x_0)^2 f''(x_0) + O \tag{3}$$

And the integral can be approximated by

$$\int_a^b \exp[-Mf(x)]dx \approx \exp[-Mf(x_0)] \int_{-\infty}^{\infty} \exp\left[-\frac{(x - x_0)^2}{2(Mf''(x_0))^{-1}}\right] \tag{4}$$

The integration on the LHS can be recognised as a standard Gaussian integral.

$$\int_{-\infty}^{\infty} \exp\left[-\frac{(x - x_0)^2}{2(Mf''(x_0))^{-1}}\right] = \sqrt{\frac{2\pi}{Mf''(x_0)}} \tag{5}$$

leaving one with the final result

$$\int_a^b \exp[-Mf(x)]dx \approx \exp[-Mf(x_0)]\sqrt{\frac{2\pi}{Mf''(x_0)}} \tag{6}$$

2 The 2 dimensinal case

We seek to approximate

$$Q = \int_{a_x}^{b_x} \int_{a_y}^{b_y} \exp[-Mf(x,y)]dxdy \tag{7}$$

say

$$\begin{aligned} f(x,y) \approx\ & f(x_0,y_0) + \\ & f_x(x_0,y_0)(x-x_0) + \\ & f_y(x_0,y_0)(y-y_0) + \\ & \frac{1}{2}(f_{xy}(x_0,y_0) + f_{yx}(x_0,y_0))(x-x_0)(y-y_0) + \\ & \frac{1}{2} f_{xx}(x_0,y_0)(x-x_0)^2 + \\ & \frac{1}{2} f_{yy}(x_0,y_0)(y-y_0)^2 + O \end{aligned} \tag{8}$$

If the first derivatives are equal to zero, the quadratic form is easily recognisable:

$$\begin{pmatrix} x-x_0 \\ y-y_0 \end{pmatrix}^T \begin{pmatrix} f_{xx} & f_{xy} \\ f_{yx} & f_{yy} \end{pmatrix} \begin{pmatrix} x-x_0 \\ y-y_0 \end{pmatrix} \tag{9}$$

And thus

$$Q \approx \exp\left[-Mf(x_0,y_0)\right] \frac{2\pi}{M(f_{xx}f_{yy} - f_{xy}f_{yx})} \tag{10}$$

3 Practical considerations

The better $f(x,y)$ is approximated by a quadratic function, and the large M is, the better the approximation is. Having an analytical solution to the location of x_0 and y_0 is desirable, as this will facilitate a quick way of obtaining the final expressions.

4 Example: Introduction of experimental errors in the refinement likelihood function

The pdf under study is

$$P(I_t; I_c) = \frac{1}{\epsilon\beta} \exp\left[-\frac{I_t + \alpha^2 I_c}{\epsilon\beta}\right] I_0 \left[\left(\frac{4\alpha^2 I_t I_o}{\epsilon^2\beta^2}\right)^{1/2}\right] \tag{11}$$

Now say that I_t is actually a random variable, for which we have a prior distribution. We get

$$P(I_o; I_c) = \int_{-\infty}^{\infty} P(I_t; I_c) P(I_o; I_t) dI_t \tag{12}$$

Although an analytical solution is available (see Pannu & Read paper), it is instructive to do this via the Laplace approximation. First of all, note that a Bessel function can be approximated by the series:

$$I_0(x) = \sum_{n=0}^{\infty} \frac{(z/2)^{2k}}{(n!)^2} \tag{13}$$

Write

$$P(I_o|I_c) = \int_0^{\infty} \frac{1}{\epsilon\beta} \exp\left[-\frac{I_t + \alpha^2 I_c}{\epsilon\beta}\right] \exp\left[\frac{(I_o - I_t)^2}{2\sigma^2}\right] \left(\sum_{n=0}^{\infty} \frac{\left(\frac{\alpha^2 I_c I_t}{\epsilon^2\beta^2}\right)^n}{(n!)^2}\right) dI_t \tag{14}$$

We interchange the summation and integration sign, without giving (or actually having) proof that the stipulated seriers is uniformly convergent on the specified integration domain. Thios results in a sum of integrals, which can be evaluated one at the time.

$$P(I_o|I_c) = \sum_{n=0}^{\infty} P_n \tag{15}$$

$$P_n = \int_0^{\infty} \frac{1}{\epsilon\beta} \exp\left[-\frac{I_t + \alpha^2 I_c}{\epsilon\beta}\right] \exp\left[\frac{-(I_o - I_t)^2}{2\sigma^2}\right] \frac{\left(\frac{\alpha^2 I_c I_t}{\epsilon^2\beta^2}\right)^n}{4(n!)^2} dI_t \tag{16}$$

The above integral suits itself for a laplace approximation, as seen below. write

$$
\begin{aligned}
f(I_t) &= \log[\epsilon] + \log[\beta] + \log[(n!)^2] \\
& \frac{I_t + \alpha^2 I_c}{\epsilon\beta} + \frac{(I_o - I_t)^2}{2\sigma^2} + \\
& -n \log\left[\frac{\alpha^2 I_c I_t}{\epsilon^2 \beta^2}\right] \qquad (17)
\end{aligned}
$$

The first and second derivatives are equal to

$$
\begin{aligned}
f'(I_t) &= \frac{1}{\beta\epsilon} - \frac{n}{I_t} - \frac{I_o - I_t}{\sigma^2} \qquad (18) \\
f''(I_t) &= \frac{n}{I_t^2} + \frac{1}{\sigma^2} \qquad (19)
\end{aligned}
$$

The roots of the first derivative are given by

$$
I_t(\hat{\pm}) = -\frac{\frac{1}{\epsilon\beta} - \frac{I_o}{\sigma^2}}{2/\sigma^2} \pm \frac{\sqrt{\left(\frac{1}{\epsilon\beta} - \frac{I_o}{\sigma^2}\right)^2 + \frac{4n}{\sigma^2}}}{2/\sigma^2} \qquad (20)
$$

As we are only interested in the maximum of $f(I_t)$, only one of the solutions is of our interest. The solution will be that for which

$$
f'(\hat{I}_t - \delta) < f'(\hat{I}_t + \delta) \qquad (21)
$$

In order to indentify the proper solution, we write

$$
\begin{aligned}
g(\hat{x}_+ + \delta)(\hat{x}_+ + \delta) &= a(\hat{x}_+ + \delta)^2 + b(\hat{x}_+ + \delta) + c \qquad (22) \\
g(\hat{x}_+) &= 0 \qquad (23) \\
\hat{x}_+ &= \frac{-b + \sqrt{b^2 - 4ac}}{2a} \qquad (24)
\end{aligned}
$$

we also have

$$
\begin{aligned}
g(\hat{x}_- + \delta)(\hat{x}_- + \delta) &= a(\hat{x}_- + \delta)^2 + b(\hat{x}_- + \delta) + c \qquad (25) \\
g(\hat{x}_-) &= 0 \qquad (26) \\
\hat{x}_- &= \frac{-b - \sqrt{b^2 - 4ac}}{2a} \qquad (27)
\end{aligned}
$$

For our case, we have $a > 0$ and the determinant (the square root) exists. We also know that $|b| \leq \sqrt{b^2 - 4ac}$ holds. It is then easy to show that $x_- < 0$ and $x_+ > 0$.

This implicates that

$$\begin{aligned} g(\hat{x}_- + \delta)(\hat{x}_- + \delta) &< 0 \quad (28) \\ g(\hat{x}_+ + \delta)(\hat{x}_+ + \delta) &> 0 \quad (29) \\ g(\hat{x}_- + \delta) &> 0 \quad (30) \\ g(\hat{x}_+ + \delta) &< 0 \quad (31) \\ & \quad (32) \end{aligned}$$

As the sign of a derivative around a maximum should change from positive to negative, the solution sought after in the laplace approximation is allways

$$\hat{I}_t = -\frac{\frac{1}{\epsilon\beta} - \frac{I_o}{\sigma^2}}{2/\sigma^2} + \frac{\sqrt{\left(\frac{1}{\epsilon\beta} - \frac{I_o}{\sigma^2}\right)^2 + \frac{4n}{\sigma^2}}}{2/\sigma^2} \quad (33)$$

It is good to notice that $\hat{I}_t$ does nopt depend on I_c, which is nice.

The approximate value of the integral is thus equal to

$$\begin{aligned} P_n \approx \; & \frac{1}{\epsilon\beta} \exp\left[-\frac{\hat{I}_t + \alpha^2 I_c}{\epsilon\beta}\right] \exp\left[\frac{-\left(I_o - \hat{I}_t\right)^2}{2\sigma^2}\right] \times \\ & \frac{\left(\frac{\alpha^2 I_c \hat{I}_t}{\epsilon^2\beta^2}\right)^n}{(n!)^2} \sqrt{\frac{2\pi}{\frac{n}{\hat{I}_t^2} + \frac{1}{\sigma^2}}} \end{aligned} \quad (34)$$

Note that the distribution is not normalized after the application of the laplace approximation. In order to normalise the distribution, integrate the distribution:

$$\kappa = \int_0^\infty P_{tot}(I_c) dI_c \tag{35}$$

This integration can be done numerically.

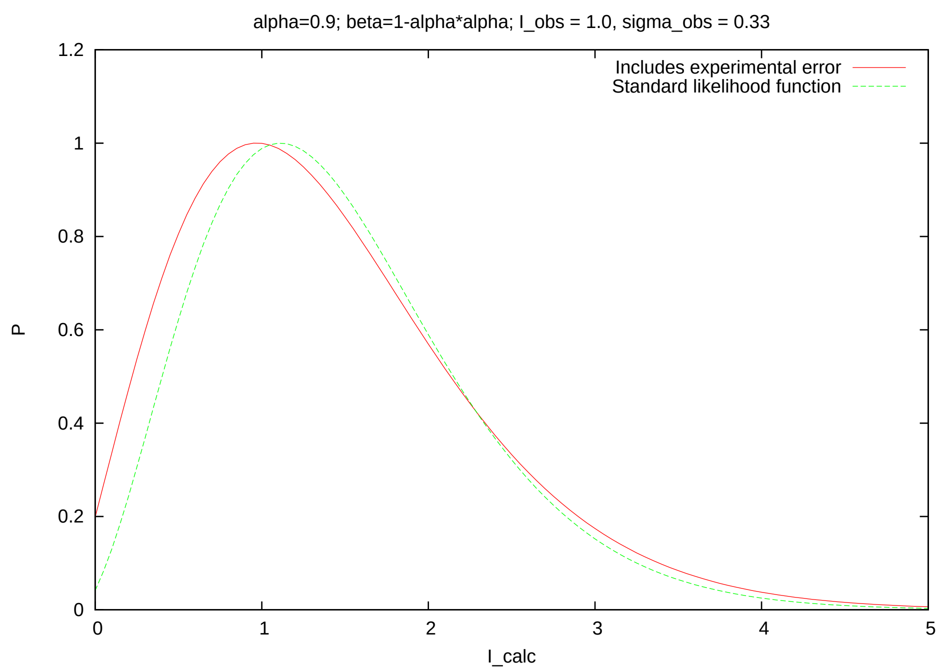
For refinement however, the following functions need to be computed:

$$Q = -\log\left[\kappa \sum_{n=0}^{\infty} P_n\right] \tag{36}$$

$$\frac{\partial Q}{\partial I_c} = \frac{\kappa \sum_{n=0}^{\infty} \frac{\partial P_n}{\partial I_t}}{\kappa \sum_{n=0}^{\infty} P_n} \tag{37}$$

$$\frac{\partial P_n}{\partial I_c} = \left(\frac{n}{I_c} - \frac{\alpha^2}{\epsilon\beta}\right) P_n \tag{38}$$

The effect of the errors on the distribution can be seen in the following fig-



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